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Quality Control Algorithms for Ocean Temperature Data

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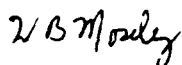
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Foreword

The Navy's mission and the performance of its weapons systems rely heavily upon knowledge of the environment in which they must operate. The amount of data available to describe the world's oceans is expanding, due primarily to the increase of remotely sensed information; but the ocean is still under-sampled. Thus, to provide an accurate depiction of the three-dimensional ocean thermal structure, we are challenged to make the best use of available observations. Satellite measurements of the ocean's surface provide us with a way to resolve mesoscale features, such as ocean fronts and eddies. Sophisticated objective analyses, such as the Optimum Thermal Interpolation System (OTIS), have been developed and implemented at the Navy's Fleet Numerical Oceanography Center. These products assure us that such information is intelligently combined with in situ data from ships, buoys, and bathythermographs. Automated quality control of these data is a key element in producing an accurate analysis product. This report focuses on those procedures, and describes the techniques used to assure that erroneous data are not negatively influencing the final product. Since OTIS results and other associated model outputs are regularly disseminated to the Fleet, improvement in the quality control of the environmental data provides the Fleet with better guidance for operational decision-making.



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Executive Summary

The Fleet Numerical Oceanography Center (FNOC) provides daily analyses of the three-dimensional ocean thermal structure both to the Fleet and to regional oceanography centers around the world. These analyses are performed on both hemispheric and regional scale grids, with resolutions as fine as 20 km in some areas. The Remote Sensing Branch of the Naval Ocean Research and Development Activity (NORDA) has been involved in assessing the impact of multichannel sea surface temperatures (MCSSTs) on these ocean thermal analyses. Specifically, NORDA has worked closely with FNOC in developing the Optimum Thermal Interpolation System (OTIS). NORDA's primary interest was to assure that the MCSSTs were properly utilized to detect and analyze mesoscale ocean fronts and eddies, with particular attention paid to how the MCSSTs were assimilated with other types of data. Through this joint effort, FNOC has successfully implemented OTIS as the operational ocean thermal analysis system for the global analysis and the Gulf Stream regional analysis.

In addition to processing and assimilating data from various sources, OTIS includes algorithms to automatically make decisions about the quality of the observations and to ignore data that are apparently erroneous. There are two basic methods of quality controlling data in OTIS. The first is the gross-error check, where observations are compared to the climatological first-guess field to assure that the data fall within reasonable ranges of the expected values. Then, groups of observations are subjected to a check for horizontal consistency, often called a "buddy check." Thus, if a particular observation cannot be corroborated by other nearby data, it is generally excluded from the analysis. This report describes the details of the automated quality control procedures in OTIS, and provides an account of the fine tuning that is necessary to optimize these techniques. The end result is a system that eliminates most of the bad data while retaining most of the valid observations, thus contributing to an improved ocean thermal analysis product.

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Quality Control Algorithms for Ocean Temperature Data

I. Introduction

Over the last two decades, we have seen dramatic improvements in our ability to describe the environment in which we live. With the advent of remotely sensed data, in particular, the world's air-ocean data base has continued to expand. As a result, we now require some of the most powerful computers in the world to process and interpret the vast amounts of available environmental data. Nevertheless, large regions of the globe remain undersampled. Not only are environmental data irregularly distributed in space and time, but they come from a variety of sensors, each with different error characteristics. Thus, increasingly sophisticated algorithms have been developed to provide objective analysis systems that can intelligently assimilate the available data. Automated error detection, while often overlooked, must be an inherent part of any such system: it is a key element in producing accurate and physically realistic analyses.

The most common analysis technique used today is the statistical method known as optimum interpolation. It was first applied to the multivariate analysis of environmental variables by Gandin (1963). Over the years, it has been adapted for use in operational meteorological analyses by the National Meteorological Center (McPherson et al., 1979), the Air Force Global Weather Center, the Canadian Recherche en Prevision Numerique (Rutherford, 1976), the European Center for Medium Range Weather Forecasts (Lorenc, 1981), the United Kingdom Meteorological Office (Lorenc, 1986), the Navy's Fleet Numerical Oceanography Center (Barker et al., 1988), and others. While optimum interpolation has also been utilized for oceanographic experiments (Bretherton et al., 1976; Freeland and Gould, 1976; White, 1977; Roemmich, 1983; Robinson and Leslie, 1985), its use has not been widespread for this particular type of application. However, the Navy has recently implemented the first operational three-dimensional ocean thermal analysis that uses the optimum interpolation methodology. That software, the Optimum Thermal Interpolation System (OTIS), replaced the previous analysis system, the Expanded Ocean Thermal Structure (EOTS) analysis (Clancy and Pollak, 1983), as the Navy's operational product at the Fleet Numerical Oceanography Center (FNOC) in Monterey, California.

The initial implementation of OTIS was for hemispheric-scale (200- to 400-km resolution) analyses only, and is referred to as OTIS 1.0. The Naval Ocean Research and Development Activity (NORDA) assisted FNOC in the development of a regional-scale version of OTIS 1.0 that can be run in various areas on a 20- to 40-km resolution grid. The regional analysis uses a feature model approach, where front and eddy positions obtained from satellite infrared and altimetry data are used to embed physically realistic fronts and eddies into the three-dimensional temperature fields (Bennett et al., 1989).

Additionally, NORDA developed another regional version of OTIS 1.0 that is capable of analyzing only sea surface temperature (SST) at even higher resolutions. This system, called SST-OTIS, can fully utilize the abundant multichannel sea surface temperature (MCSST) data from the polar-orbiting satellites. Because of the large amounts of data that must be processed and the number of grid points that must be analyzed, the SST-OTIS was designed to run on FNOC's supercomputer—the Control Data Corporation's Cyber 205. The SST-OTIS contains all the features of the regional OTIS 1.0 plus some additional capabilities. Physically, OTIS 1.0 does not need high-resolution (up to 4 km) data to resolve features on the hemispheric scale. Also, from a practical standpoint, the computer resources available to OTIS 1.0 are limited. Therefore, OTIS 1.0 averages the MCSST data to form an MCSST "superob" at each grid point prior to performing the data analysis. This procedure is neither necessary nor desirable in the high-resolution SST-OTIS. To analyze mesoscale features, such as fronts and eddies, we wanted to consider the input of each available observation.

While SST-OTIS is not a separate operational product, the ideas presented here on data quality control apply to other analysis systems, as well, and many of the suggested changes in quality control have been directly incorporated in OTIS 1.0. SST-OTIS can be executed in either hemispheric or regional mode, with the option to superob MCSST data included, so the SST-OTIS was used for all the experiments described in this paper. Hereafter, the generic OTIS is frequently referred to, unless a distinction needs to be made between the various versions of the software.

The evaluation of a data analysis scheme can take several forms. One method is to perform an objective statistical evaluation of the results. This validation is generally accomplished by comparing the analysis results at a particular point to recently obtained data that were not included in the previous assimilation (Clancy et al., 1990). Given many such comparisons, statistics can be generated to describe the accuracy of the analysis scheme. But if our goal is to somehow replicate the decisions that a human analyst would make given the same information, we should also *subjectively* evaluate how well the individual algorithms are meeting this goal. For example, the human analyst would look at several things—the data available near the grid point, the observations that were rejected as erroneous, the observations that were actually included in the analysis, and the observations having the most influence on the outcome.

The SST-OTIS was developed primarily to assure that the MCSST data were receiving the appropriate weight relative to the other data types, and that their impact on the analysis was a positive one. However, when the OTIS data-handling algorithms were scrutinized, many shortcomings were identified in the data selection and quality control procedures—shortcomings that detrimentally affected all data sources. The end result was that many good observations were actually being ignored by the analysis, and the data selected were often not the most appropriate.

Quality control of the available data is a crucial step in any analysis procedure. The choice to include or exclude even one piece of information can result in significant changes to an analysis (Thiebaux, 1980; Phoebus, 1983; Hollingsworth et al., 1985), especially if that observation is in a data-sparse region. Since much of the world's oceans are sparsely sampled, particularly at the subsurface, it is crucial that data not be discarded unnecessarily. While no objective quality control system is perfect, we strive for a system that will eliminate most of the bad observations without rejecting too many of the useful ones.

This report emphasizes the automated quality control procedures used in OTIS. A brief background of optimum interpolation is presented in Section II. Section III describes the original techniques used to objectively quality control the data in OTIS; Section IV discusses some of the problems with these methods. Section V shows experimental results that illustrate how changes in the quality control algorithms greatly decrease the incidence of data rejection. Section VI suggests areas where further improvements in quality control can still be made. The problems with the data selection algorithms have been discussed in a separate report (Phoebus, 1988).

II. Background Theory

The application of optimum interpolation to data analysis is described in detail by Bergman (1979) and Lorenc (1981). The particular equations and notations used in OTIS are given by Clancy et al. (1989). In optimum interpolation, the analyzed variable is obtained from a linear combination of the available data, with weights assigned to each observation in such a way as to minimize the analysis error in a least-squares sense. In OTIS, the observations are converted to anomalies from the first-guess field, so that the analyzed temperature is actually computed as a correction to the first-guess field (usually climatology). Thus, given a group of N observations, the analyzed temperature at grid point k is given by

$$T_k^a = T_k^c + \sum_{i=1}^N \alpha_{ik} (T_i^o - T_i^c), \quad (1)$$

where T_k^c is the first-guess temperature at the grid point, T_i^c is the first guess interpolated to the location of the i th observation, T_i^o is the observed temperature of the i th observation, and the weight assigned to the i th observation is given by α_{ik} .

The set of weights is chosen to minimize the analysis error, and is obtained by solving the set of linear equations

$$\eta_{ik} = \sum_{j=1}^N (\eta_{ij} + \delta_{ij} \lambda_i^o) \alpha_{jk}, \quad \text{for } i = 1, 2, \dots, N, \quad (2)$$

where η_{ik} is the correlation between the observation and the analyzed temperature at the grid point, the η_{ij} are the autocorrelations between observation i and every other observation j , λ_i^o is the noise-to-signal ratio for observation i , and δ_{ij} is the Kronecker Delta function, defined as

$$\begin{aligned} \delta_{ij} &= 1, & \text{for } i = j, \\ \delta_{ij} &= 0, & \text{for } i \neq j. \end{aligned} \quad (3)$$

The correlation function used in OTIS is the Gaussian function

$$\eta_{ij} = \exp \left[- \left(\frac{\Delta x_{ij}}{AX_k} \right)^2 - \left(\frac{\Delta y_{ij}}{BY_k} \right)^2 - \left(\frac{\Delta t_{ij}}{CT_k} \right)^2 \right], \quad (4)$$

where Δx_{ij} , Δy_{ij} are the east-west and north-south distances between the two locations, Δt_{ij} is the time

difference between the two observations, and AX_k , BY_k , and CT_k are the E-W, N-S, and time correlation scales appropriate to the region of interest. The correlation η_{ik} can be evaluated using the same equation, where location j becomes the location of grid point k , and Δt_{ik} is the age of the observation. Figure 1 illustrates how the correlation changes with distance from the grid point, assuming $\Delta t_{ik} = 0$ and AX_k is twice as large as BY_k . Figure 2 shows how the correlation decreases as the observations age, for various values of CT_k . The total correlation can be thought of as the product of these two separate functions.

The set of N observations influencing the analysis at a particular point are those observations that are the most highly correlated with the analyzed value at the grid point. The details of the data selection algorithms are given by Phoebus (1988). Basically, the

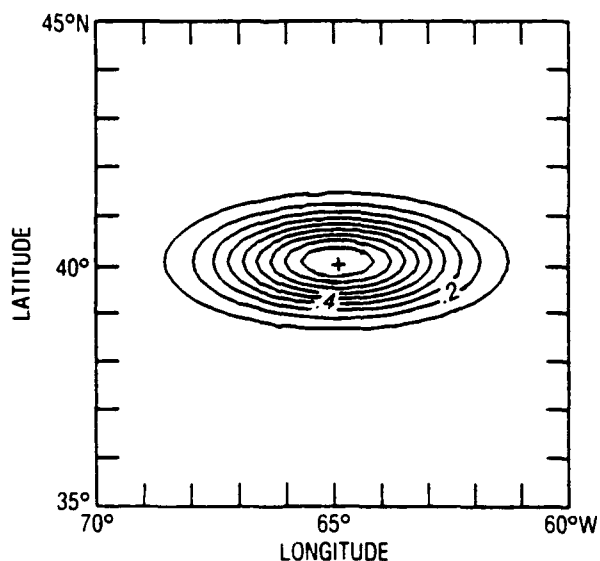


Figure 1. Spatial correlation function for $AX_k = 200$ km and $BY_k = 100$ km. Contours are plotted from 0.1 to 0.9 at intervals of 0.1. The grid point is located at the center of the figure.

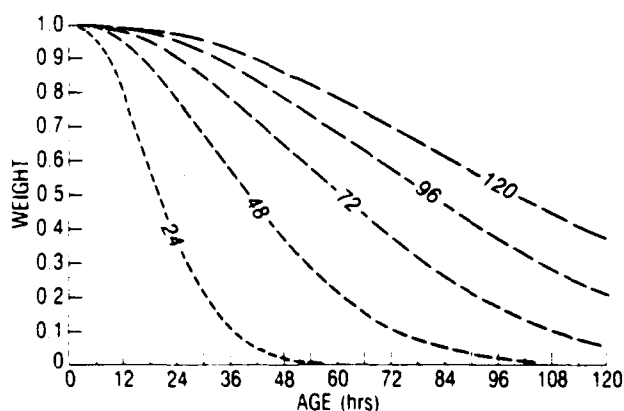


Figure 2. Time correlation function for various values of CT_k , given in hours.

total correlation η_{ik} is evaluated for each observation within a certain distance of the grid point—a distance that is also a function of AX_k and BY_k . The 15 most highly correlated observations are retained for input into the analysis. If fewer than 15 are available, then the entire set is used.

To assure that the selected observations contain valid information, some means of quality controlling the data must be provided. Before the days of computerized analyses, the human analyst would survey the data and, based on his or her experience and knowledge of the physical variables being analyzed, would decide to reject or ignore certain information. This decision was usually made by comparing an observation to other nearby data or to values considered "reasonable" for that particular parameter. Because of the large volume of global environmental data being processed today, it has become necessary to automate almost all of the data quality control procedures.

At FNOC and other operational centers, most of the quality control is left to the individual user. That is, the data receive very little checking before being placed in the data archive files. The argument for this approach is that the validity of a certain piece of data is somewhat dependent upon the particular application. For example, an expendable bathythermograph (XBT) deployed in an oceanographic eddy provides very useful information for a mesoscale analysis. However, for a hemispheric-scale analysis, such an observation represents a feature that cannot be resolved and is essentially noise. For the latter product, the observation should be rejected. The observation is not erroneous, but neither is it applicable to the particular problem. Therefore, each operational product must have its own rather intensive quality control procedures.

III. Original Quality Control Algorithms in OTIS

The quality control procedures in OTIS are composed of three separate steps. First, observations with physically unrealistic values are ignored. Next, each observation is subjected to a "gross-error check," where it is compared to climatology (the first-guess field). Finally, each observation is compared to other nearby observations in a procedure known as a horizontal consistency check, or "buddy check." These procedures are not unique to OTIS. They have been used successfully in the meteorology community for many years (Daly et al., 1985).

Observations that are outside the range of normal ocean temperatures are rejected as the data files are initially read into OTIS. Thus, reports of less than -2°C or greater than 40°C are screened from the analysis. Such values often occur due to transmission or recording errors.

The gross-error check is performed at the time the anomalies are formed. If any observation deviates from climatology by more than a fixed amount, then it is excluded from the data set. Presently in OTIS, this tolerance is constant everywhere on the grid. Data anomalies that exceed the predefined tolerance are eliminated and never used in the analysis.

The buddy check is more an integral part of the analysis, because it is performed at each point only after the (up to) 15 most highly correlated observed anomalies have been selected. Based upon the work of Bergman (1979), the buddy check compares the temperature difference between two anomalies to some tolerance that is a function of the autocorrelation of the two observations. In mathematical terms, the relationship that must be satisfied is

$$|(T_i^o - T_i^c) - (T_j^o - T_j^c)| \leq (a - b\eta_{ij})\sigma_k^c, \quad (5)$$

where a and b are empirical constants, η_{ij} is the autocorrelation computed from equation (4), and σ_k^c is the sample standard deviation from the previous analysis. If the absolute temperature difference between the anomalies $T_i^o - T_i^c$ and $T_j^o - T_j^c$ is greater than the expression on the right-hand side of equation (5), then a toss flag is set against each of the two observations to indicate that they are not in agreement. The value of this toss flag is 1.0.

After each possible pair of observations at the grid point has been compared in this way, the total number of toss flags set against each observation is checked. Any observation with less than 2.0 toss flags is automatically saved. Otherwise, the observed anomaly with the greatest number of toss flags is removed from the set of data selected for this grid point; it is not removed from the data set as a whole. Subsequently, any flags that were set on other observations by the rejected observation are also removed. Each remaining pair of observations is then compared again using equation (5), and the next observation receiving the most toss flags is rejected.

This iterative process continues until no observation has a total of 2.0 or more toss flags, or until only two observations remain. Because only observed anomalies with 2.0 or more toss flags can be rejected, at least two other observations must disagree with the questionable report before it can be rejected. Thus, one bad report cannot cause good data to be eliminated.

The buddy check is described schematically in Figure 3. The abscissa is the absolute temperature difference between two observed anomalies. The ordinate is the autocorrelation between the same two data points. The plotted line represents the dividing line between a "toss" or "no toss" situation. If the two observations in question have a temperature difference that is greater than the tolerance for that

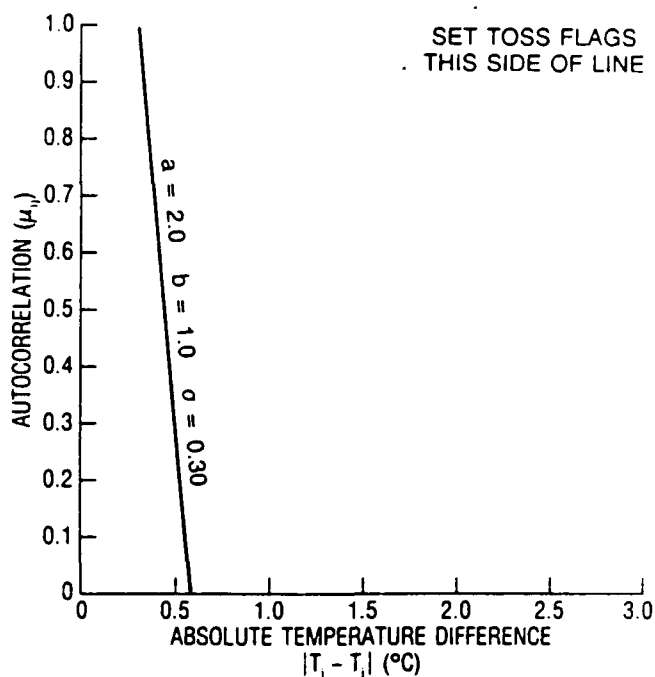


Figure 3. Functional illustration of the division between setting or not setting toss flags on a pair of observations being considered by the buddy check.

particular autocorrelation (in other words, to the right of the line), then toss flags are set on both anomalies. The diagram also makes it easy to see that as the correlation between the observations increases, the allowed temperature difference between them decreases. Thus, in general, data that are closer together in space and time are expected to agree in value more than observations that are farther apart.

The particular values chosen for a , b , and σ_k^c affect the slope and intercept of the dividing line. Since σ_k^c represents the mean departure of the observations from climatology in the previous analysis, a larger value of σ_k^c reflects the fact that a higher variance is expected in the data anomalies. For example, an increase in σ_k^c from 0.30 to 0.80 moves the entire dividing line to the right, thus increasing the overall tolerance for temperature deviations between neighboring observations (Fig. 4), with more of an increase evident for the less correlated data. Similarly, adjusting the values of a and b from 2.0 and 1.0 to 3.0 and 1.5, respectively, while holding σ_k^c constant, also results in fewer toss flags being accessed (Fig. 5). Since a and b are empirical constants, they can be thought of as tuning parameters whose values can be adjusted to further restrict or loosen the tolerance on flagging data.

IV. Discussion of Quality Control Problems

The specific quality control algorithms that were initially utilized in OTIS have been described. During

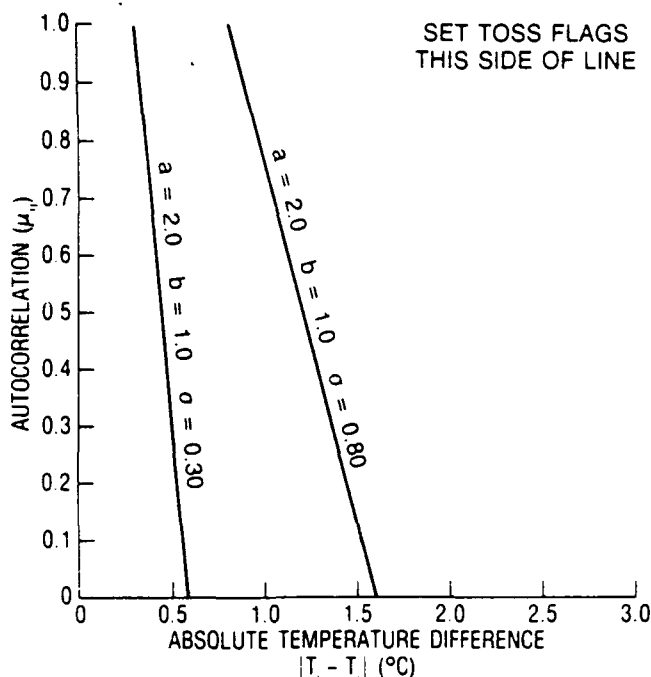


Figure 4. Illustration of how a larger value of σ_k^2 in Equation (5) increases the temperature difference allowed between two observations before toss flags are set by the buddy check.

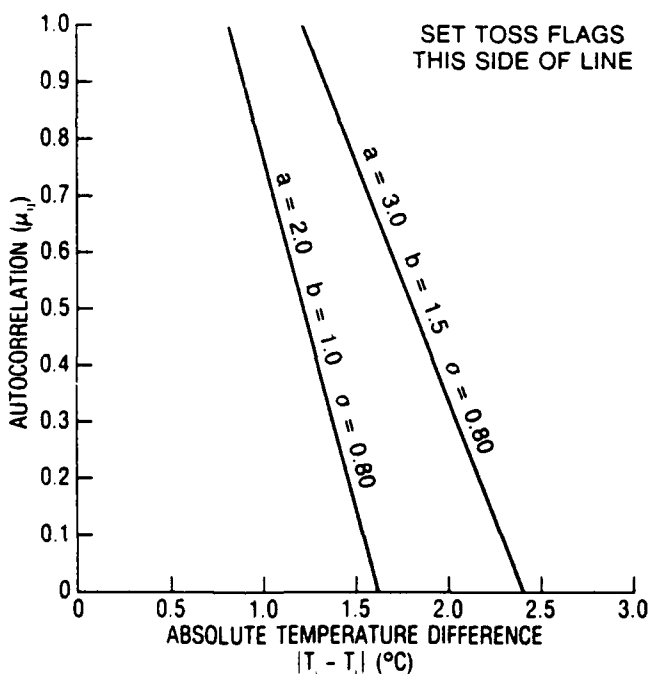


Figure 5. Illustration of how larger values of a and b in Equation (5) increase the temperature difference allowed between two observations before toss flags are set by the buddy check.

the development of the SST-OTIS at NORDA, it became apparent that large amounts of data were being rejected, and the resulting analysis closely resembled climatology. Further investigation showed similar problems in the global three-dimensional OTIS 1.0, as well. Therefore, an extensive study of the quality

control algorithms was undertaken, and several modifications were made as a result.

First, the gross-error check was rejecting all temperature anomalies greater than 5°C , which proved excessive. The purpose of the gross-error check should be to reject observations that are obviously erroneous, that is, those observations outside the range of reasonable values for a specific location at a given time of the year. Since mesoscale events are sampled, even though they may not be analyzed, deviations of 5° from climatology would not be at all unusual in the vicinity of fronts and eddies. Therefore, it is premature to reject such observations in the gross-error check. It would be preferable to leave them in and allow them to be interrogated by the buddy check. At NORDA's suggestion, FNOC agreed to increase the tolerance from 5° to 7°C for the hemispheric analysis.

A recent occurrence of very cold water in the eastern equatorial Pacific made even the 7°C tolerance seem too restrictive for some events. For example, MCSST data from May and June 1988 in the region from 100° to 160°W indicated anomalies that approached the limits of the gross-error checks. Figures 6a and 6b compare the first-guess SSTs to the values of the MCSST superobs at the same locations for May 9, 1988. Differences of more than 6°C can be seen near 0.5°N and 134.0°W . The strengths of these anomalies were verified by other independent sources of information. This extremely cold upwelling event, coupled with NORDA's observation of gaps in the MCSST data along the equator, resulted in changes in the methods used to quality control MCSSTs at the National Environmental Satellite Data and Information Service (NESDIS). NESDIS increased their gross-error check tolerance from 7° to 10°C to assure that they were not disregarding valid MCSSTs in this area. NORDA recommended that FNOC consider similar changes in the hemispheric OTIS gross-error check, at least in certain regions.

For regional analyses such as the SST-OTIS, a case can be made for allowing larger anomalies to pass the gross-error check. For example, a slight shift in the position of an eddy or the north wall of the Gulf Stream can result in extremely large, but nevertheless valid, anomalies. In SST-OTIS, the gross-error tolerance was set initially at 7°C , but has been increased even more, based on data from the 30 March 1988 analysis. Figure 7 indicates the position of the north wall in the first-guess field on that day. A large number of MCSSTs are available in the outlined area off Cape Hatteras (Figs. 8 and 9). The 15°C isotherm, which is often indicative of the surface position of the north wall, is sketched from this data. Notice the two meanders in this isotherm. Judging from the MCSST data, the north wall in the first-guess field was displaced

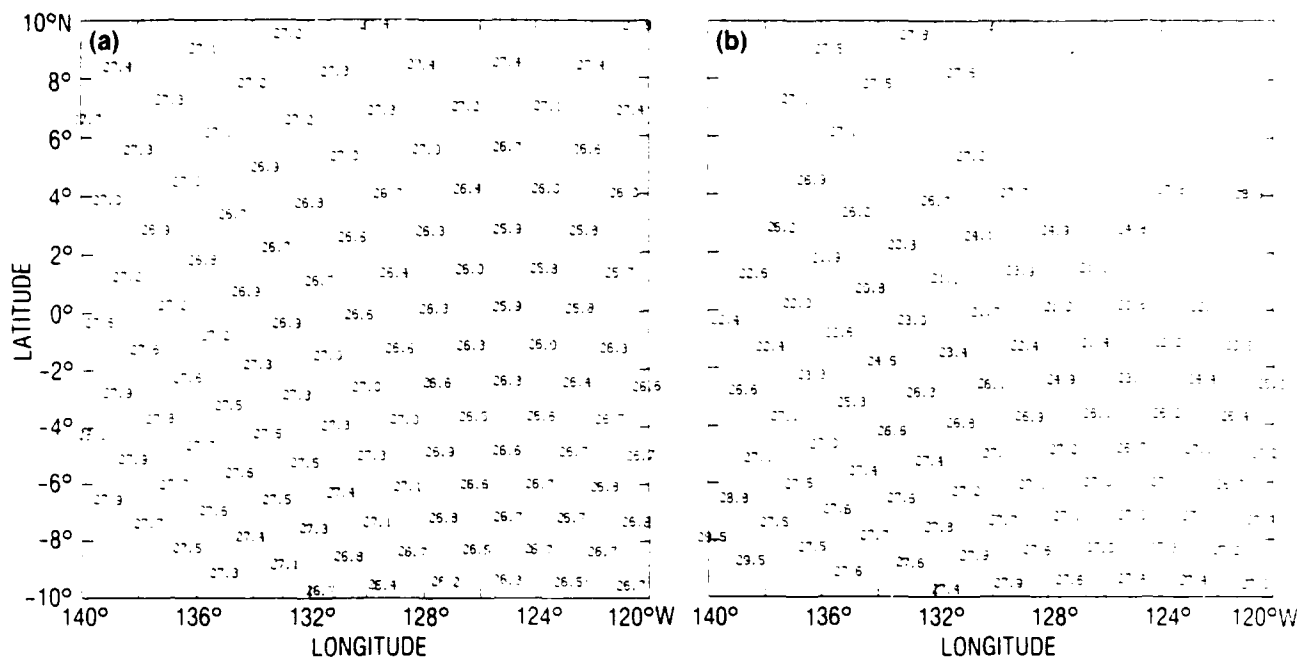


Figure 6. (a) Climatological first-guess SSTs for May 9, 1988, at grid points in the eastern equatorial Pacific. (b) MCSST superob temperatures for May 9, 1988, at grid points in the eastern equatorial Pacific.

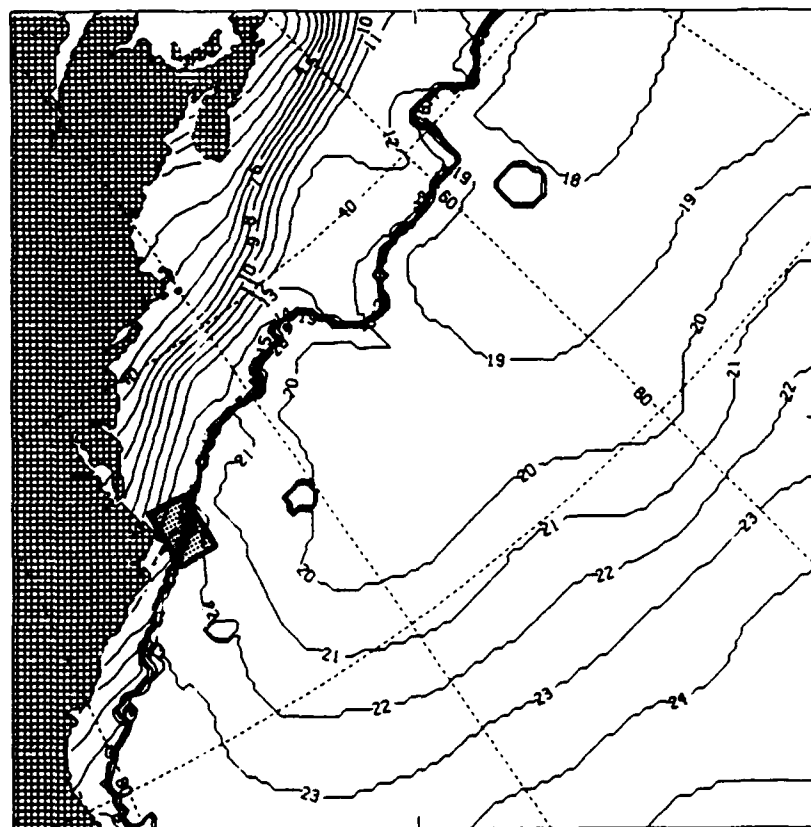


Figure 7. Climatological first-guess SST field for March 30, 1988, with the Gulf Stream front and eddies embedded.

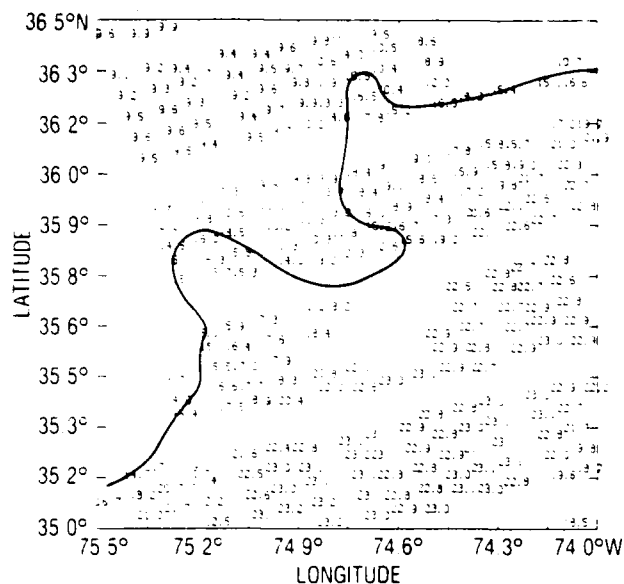


Figure 8. MCSST observations for March 30, 1988, just off the coast of Cape Hatteras. The 15°C hand-analyzed isotherm is shown.

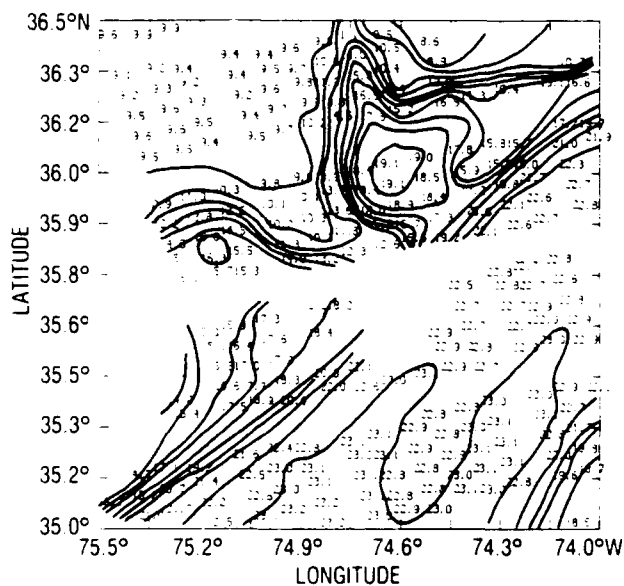


Figure 9. Hand-drawn analysis of the MCSST data shown in Figure 8. Note the position of the Gulf Stream as indicated by the large gradient in the MCSST data.

too far to the southeast. Although the climatology in the area just northwest of the first-guess position of the Gulf Stream was approximately 14°C, the data indicated that the true temperature in the region was more like 22° or 23°C. However, the gross-error check rejected these observations because their anomalies were too large.

Figure 10a provides a closer look at the position of the north wall of the Gulf Stream in the first-guess SST field just off Cape Hatteras. The 15°C isotherm is highlighted. Two separate analyses were run; both used

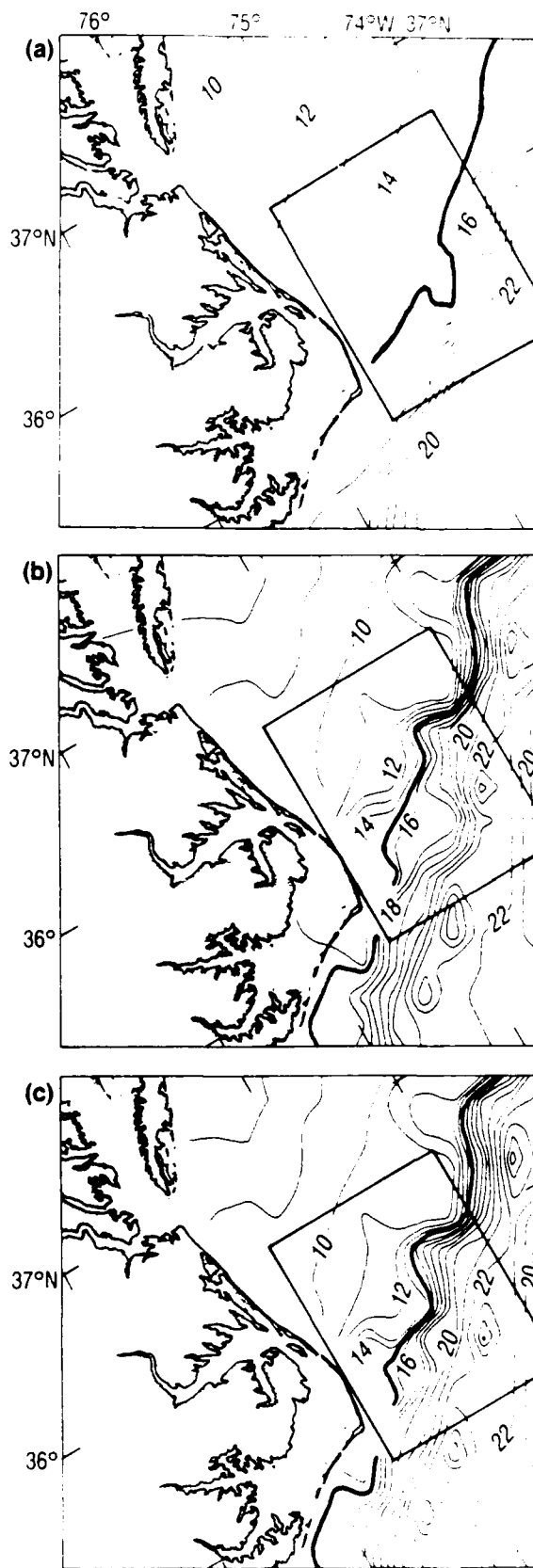


Figure 10. Position of the Gulf Stream front just off Cape Hatteras on March 30, 1988. Contours are every 1°C. (a) Climatological first-guess. (b) SST analysis with gross-error tolerance of 7°C. (c) SST analysis with gross-error tolerance of 10°C.

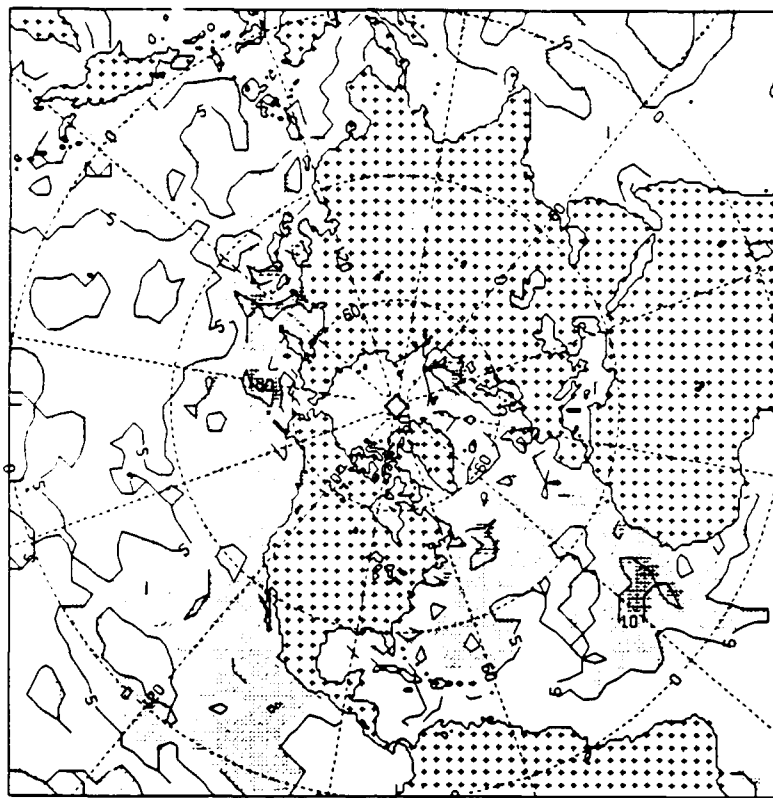


Figure 11. Shaded areas represent grid points where the buddy check was rejecting at least one-third of the selected observations.

the same buddy check algorithms. The only difference was the value assigned to the gross-error tolerance. In the original analysis, many of the 8° and 9°C anomalies were eliminated by the gross error check, resulting in the analyzed front shown in Figure 10b. When the gross error tolerance was increased from 7° to 10°C, most of these MCSST observations were retained. Furthermore, the buddy check did not reject them, since each group had numerous supporting observations. The resulting analysis repositioned the front more effectively (Fig. 10c), better reflecting the true position of the north wall that is readily seen in the raw MCSST data (Fig. 9).

Second, the original buddy check, as described, was also rejecting far too much data. In the hemispheric analysis, it was not uncommon for more than 30% of the selected observations to be rejected. In other words, 15 observations would be selected for the analysis at a particular grid point, but of those 15, five or more would be rejected. Figure 11 illustrates just how widespread the problem was. The shaded areas are the grid regions where at least one-third of the data points were rejected for the case of August 3, 1987. There were obviously not that many bad observations, so the fault was clearly with the buddy check algorithms.

The National Meteorological Center (NMC) had similar problems when they first implemented Bergman's optimum interpolation analysis scheme

and buddy check in the late 1970s. Since that time, they have made many modifications to the original algorithms (Kistler and Parrish, 1982; Phoebus, 1983; Dey and Morone, 1985; DiMego et al., 1985). The result is a buddy check with more nuances and details than the original, but one that rejects fewer good observations. Many of these ideas were easily incorporated into OTIS for testing and evaluation.

For example, rather than set only *toss* flags when two observations disagree, *keep* flags can also be set for a pair of observations that corroborate one another (Kistler and Parrish, 1982). Schematically, this would be represented by the area left of the plotted line in Figure 3. Once all data pairs are compared and all flags set, the iterative procedure that rejects data is designed to always keep any anomaly that has at least 2.0 keep flags, regardless of the number of toss flags it received. In this way, any observation that disagrees with two or more other observations can only be tossed if there are not at least two observations that support it. Such a system obviously rejects fewer observations, but fails to achieve the desired result in one situation. If two groups of observations within the data search area are not in agreement (one group of data is erroneous), but each group contains at least three observations that corroborate one another, no data will be rejected. Such a situation could occur, for example, given co-located

day and night swaths of satellite data, or given a swath of satellite data in the vicinity of a frequently reporting buoy or ship.

To prevent the scenario described above, the flagging procedure can be further modified. Thus, when two observations disagree, rather than set toss flags on both of them, other information can be used to determine which of the two is more likely in error. The typical instrument error for each type of observation is available as normal input to the optimum interpolation scheme. These errors can be used to assign a flagging hierarchy to the various data types (Phoebus, 1983). Then, when two observations disagree, only the lower quality observation is flagged. If the two observations are of the same type, then the one that is less correlated with the grid point value is flagged. The relative quality assigned to each data type is given in Table 1. Keep flags are still set on both observations if they corroborate one another.

A further refinement has been made to the flagging procedure at NMC (DiMego, pers. comm.). Rather than use a value of 1.0 for each toss and keep flag, the autocorrelation of the two points being compared is used. This value would be equal to 1.0 for two observations that are co-located and taken at the same time. Normally, the flag value would be less than 1.0. This use of the autocorrelation is very appealing, for it essentially gives greater weight to flags set by observations that are closer in space and time to the observation being checked. Because it would normally take more than two observations to accumulate a total of 2.0 flags, the limits placed on the number of toss and keep flags should probably be reduced. For example, retain all observations that received at least 1.5 keep flags and reject observations that received

more than 1.5 toss flags and fewer than 1.5 keep flags. These numbers may be altered to find the particular values that work best for each application.

V. Experimental Results

The ideas suggested were applied to the OTIS buddy check in an attempt to retain more data in the analysis. The results of five experiments made with the hemispheric SST-OTIS are presented in the form of histograms in Figures 12 and 13. The first set of histograms, shown in Figure 12a-12e, portray how many of the (up to) 15 selected observations are rejected, and at how many grid points each situation occurs. The hemispheric OTIS grid contains 3969 grid points, 2754 of which are over water. Thus, when OTIS used the original buddy check to quality control the data for August 3, 1987, 308 grid points tossed 5 of the original 15 data points, while 277 grid points rejected 6 of the selected observations, and so on (Fig. 12a). All totaled, there were 1417 grid points that eliminated 5 or more observations. Thus, 51% of the analysis points rejected at least 33% of the data that normally would have been included in the analysis. It is especially disturbing that a significant number of grid points ignored more data than they used.

To add another perspective to the extent of the problem, for this particular SST analysis there were 374 XBTs, 5261 ship/buoy reports, and 1862 MCSST superobs. Thus, less than 7500 total observations were available to describe the surface temperature of the world's oceans. Yet, the original buddy check rejected 3951 of these observations (Table 2) at least once. This is more than half of the data.

Table 1. Instrument error assigned to each data type.

RELATIVE WEIGHT	DATA TYPE	HEMISPHERIC SST-OTIS	REGIONAL SST-OTIS	HEMISPHERIC OTIS 1.0
1	XBT	0.2°C	0.2°C	0.2°C
2	MCSST	0.7°C	0.7°C	0.7°C
3	DRIFTING BUOY	1.0°C	1.0°C	2.3°C ¹
4	FIXED BUOY	1.0°C	1.0°C	2.3°C
5	COASTAL MARINE	1.0°C	1.0°C	2.3°C
6	SHIP	2.3°C	2.3°C	2.3°C

¹ OTIS 1.0 does not distinguish between ship and buoy reports.

Table 2. Total number of observations tossed by the buddy check.

	HEMISPHERIC SST-OTIS	REGIONAL SST-OTIS
CASE 1	3951	2544
CASE 2	2996	1352
CASE 3	634	223
CASE 4	562	209
CASE 5	773	193

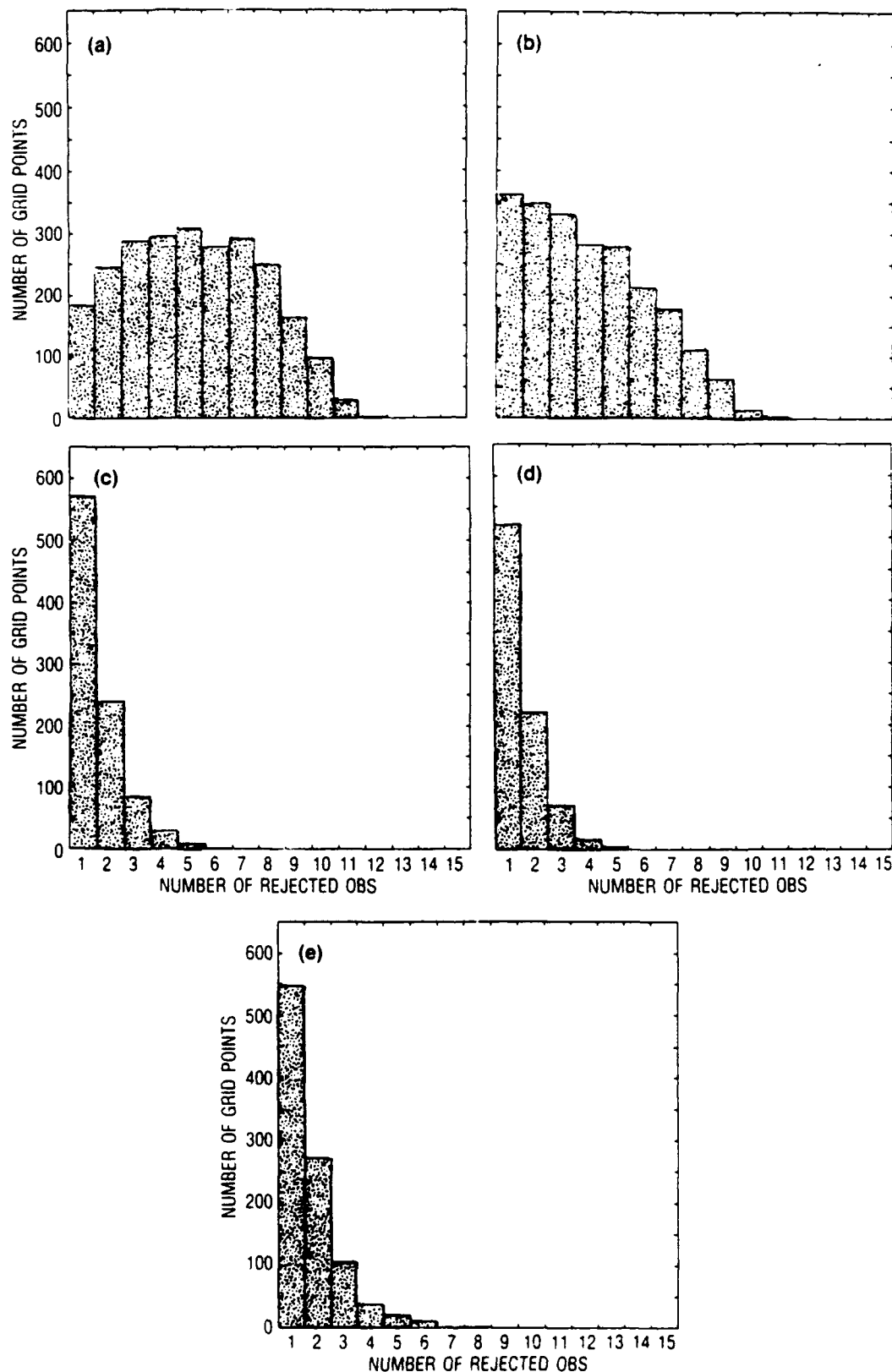


Figure 12. Histograms illustrating how many of the 15 selected observations were rejected by the buddy check, and at how many grid points this situation occurred for the northern hemispheric analysis on August 3, 1987. (a) Original buddy check; (b) constants a and b increased by 50%; (c) keep flags, as well as toss flags, set on both observations; (d) keep flags set on both observations, but toss flags set on only one; (e) autocorrelation used as flag value and flag limits reduced to 1.5.

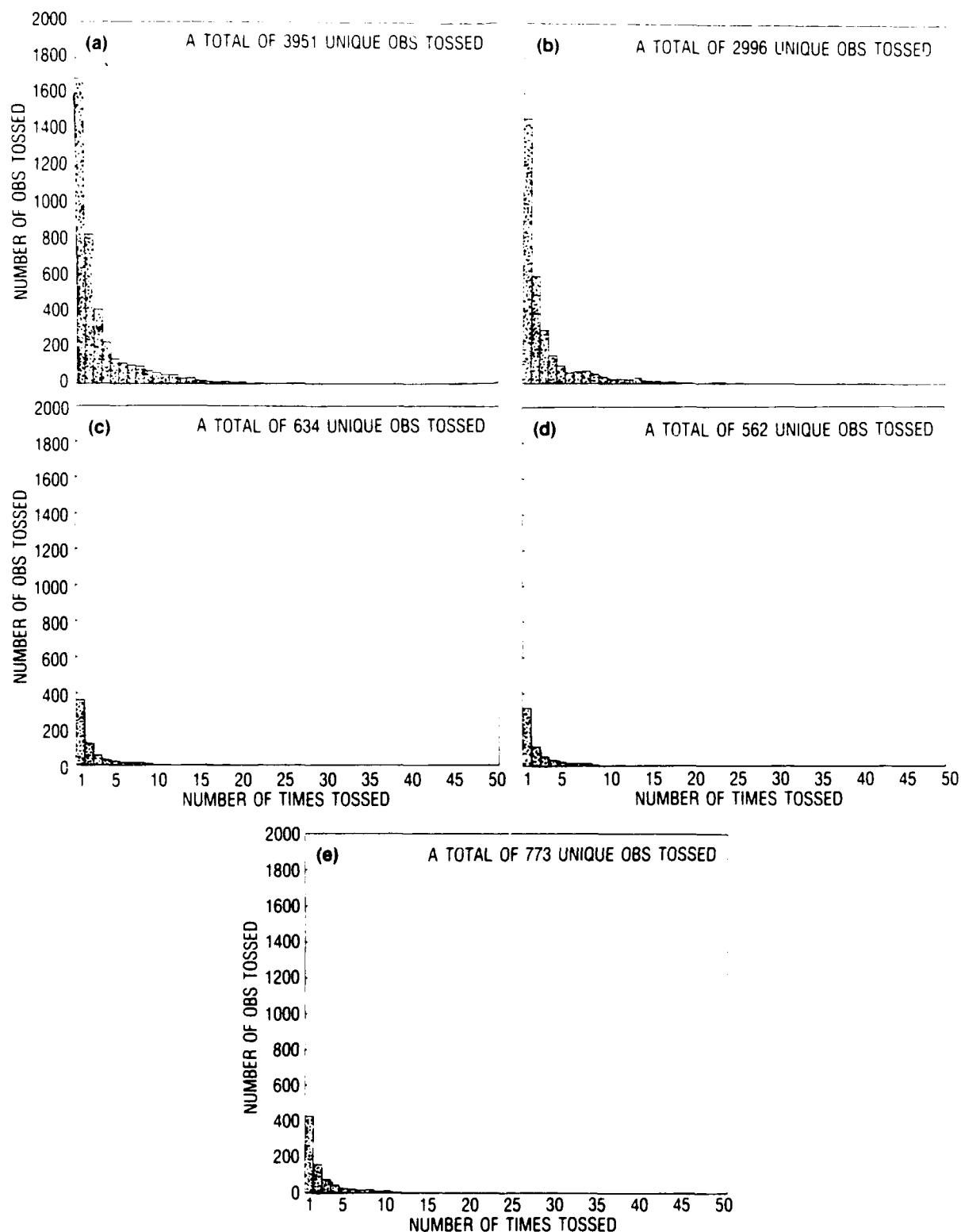


Figure 13. Histograms illustrating how many times a particular observation was rejected, and the number of observations in each of these categories for the northern hemispheric analysis on August 3, 1987. (a) Original buddy check; (b) constants a and b increased by 50%; (c) keep flags, as well as toss flags, set on both observations; (d) keep flags set on both observations, but toss flags set on only one; (e) autocorrelation used as flag value and flag limits reduced to 1.5.

The first modification made to the buddy check was simply to increase the difference that would be allowed between two temperature anomalies before toss flags would be set. This change is easily accomplished by increasing the values of the constants a and b in Equation (5). Initially set at 2.0 and 1.0, respectively, the values of a and b were increased by 50% to 3.0 and 1.5, resulting in the tolerance illustrated in Figure 5. The decrease in the number of observations rejected by the buddy check is illustrated in Figure 12b. Notice, in particular, the shift toward lower numbers of rejected observations, even though there are still grid points that are tossing the majority of the selected observations.

The next step was to include the use of keep flags as well as toss flags when the data were compared. Thus, when two anomalies disagreed, by the standards of Equation (5), toss flags of value 1.0 were set on both data points. Similarly, when the two anomalies were in agreement, keep flags of value 1.0 were set on both observations. Furthermore, any observation corroborated by at least two other observations in the group could not be rejected under any circumstances. Observations with more than 2.0 toss flags and less than 2.0 keep flags were removed, following the iterative procedure described in the previous section. The results were fairly dramatic, as illustrated in Figure 12c. With the addition of keep flags, very few grid points tossed as many as five observations, with most grid points only rejecting 1 or 2 data points. This situation appears to be much more realistic. Furthermore, the total number of observations rejected has been reduced from 3951 originally to 634 in this case.

The fourth experiment involved modifying the flagging procedure so that while keep flags were set on both observations, a toss flag would be set on only one of the conflicting data pair. Thus, we are assuming that if two observations disagree, one of them is likely to be correct and only one of them is in error. We further assume that the observation in error is the one from the source with traditionally the highest instrument error. If the data pair come from the same instrument type, then the observation that is the least correlated with the grid point is assumed to be the erroneous one. This change results in fewer observations rejected in each numerical category (Fig. 12d).

The final case makes the same assumptions as the previous experiment. The only difference is that the flag values are reduced from a value of 1.0 to the value of the autocorrelation between the pair of observations being compared, while the maximum tolerances on keep and toss flags are reduced from a total of 2.0 to a total of 1.5. Thus, any anomaly receiving at least 1.5 keep flags is always retained, while anomalies receiving 1.5 or more toss flags and less than 1.5 keep flags are removed. This modification (Fig. 12e) actually

seems to produce worse results than the previous case. While the basic idea of using the autocorrelation is a sensible one, the choice of the limiting value of 1.5 is arbitrary, and may not be the most suitable.

Figure 13 shows another set of results from the five hemispheric buddy check experiments. Since the data search radii generally encompass several grid intervals, each observation is included in the search area for more than one grid point, and is thus interrogated by the buddy check numerous times. If an observation is in error, then we would expect it to be tossed by nearly every grid point that selects it. Figure 13a illustrates the number of data anomalies that are rejected in the original buddy check by 1, 2, 3, ..., 50 grid points. Notice the large number of observations that are rejected only once. This rate is a strong indicator that the buddy check is not performing as desired.

The modified buddy check algorithms used in cases 2-4 result in both a reduction of the total number of observations rejected (Table 2) and of the number of observations rejected only once or twice (Fig. 13b-d). The improvement is especially noticeable between experiment 2 and 3, due to the addition of keep flags in the buddy check process. Again, case 5 results (Fig. 13e) are not as favorable as the preceding experiment.

In addition to summarizing the results at all grid points, each experiment also tracked the performance of the buddy check at specified diagnostic grid points. Each of the diagnostic points selected 15 observations, in the form of anomalies or residuals, for input to their respective analyses. The number of these residuals rejected at each diagnostic point for each of the 5 cases is shown in Table 3. The largest gains are made between case 2 and case 3, due to the addition of keep flags.

Special attention was paid to which particular residuals were rejected at each point. For example, consider the first diagnostic point, located in the equatorial Pacific at 1.0°N , 151.0°W . The selected temperature residuals are plotted in Figure 14a. None of the values appear particularly out of place, but the original buddy check rejected five of these data points (Table 4). Perhaps the most anomalous of the group is the 1.7°C residual at 2.1°N , 148.6°W . But the 1.7°C residual is computed from an MCSST superob, while the nearby 2.2° and 2.9°C residuals are from XBTs. Since the data are from different sources, we would not necessarily expect extremely close agreement. If all these residuals are allowed to remain in the analysis, as they are in cases 3-5, then the optimum interpolation scheme will weight the different data types appropriately. Notice in Table 4 that the analyzed anomaly changes only slightly from case to case, regardless of which data are rejected.

The diagnostic point located at 45.9°N , 61.6°W , however, presents a more complex situation. This grid point is located in a dynamically active region, which

Table 3. Number of residuals rejected at diagnostic points.

NORTHERN HEMISPHERE OTIS ANALYSIS 3 AUG 87					
	1.0°N 151.0°W	11.2°N 118.7°W	13.3°N 228.2°W	42.9°N 26.0°W	45.9°N 61.5°W
CASE 1	5	8	6	8	10
CASE 2	2	5	6	5	9
CASE 3	0	1	0	0	3
CASE 4	0	1	0	0	2
CASE 5	0	1	0	0	5

Table 4. Quality control of residuals at 1.0°N, 151.0°W.

LAT (°N)	LON (°W)	RESID (°C)	DATA TYPE	REJECTED				
				CASE 1	CASE 2	CASE 3	CASE 4	CASE 5
0.98	150.97	2.18	MCSST					
1.56	152.76	1.82	MCSST	•				
0.35	149.23	2.18	MCSST					
2.10	148.55	1.72	MCSST	•				
-0.21	153.30	2.87	MCSST					
-0.76	151.57	2.89	MCSST					
2.77	150.35	2.11	MCSST					
0.22	151.72	2.66	XBT					
2.28	147.55	2.90	XBT					
1.38	146.80	2.03	MCSST	•				
0.29	155.07	2.87	MCSST					
-0.33	147.52	2.28	MCSST					
-1.36	149.86	3.28	MCSST	•	•			
2.44	148.70	2.19	XBT					
2.10	155.90	1.27	SHIP	•	•			
ANALYZED	RESIDUAL	CORRECTION	(°C)	2.19	2.14	2.20	2.20	2.20

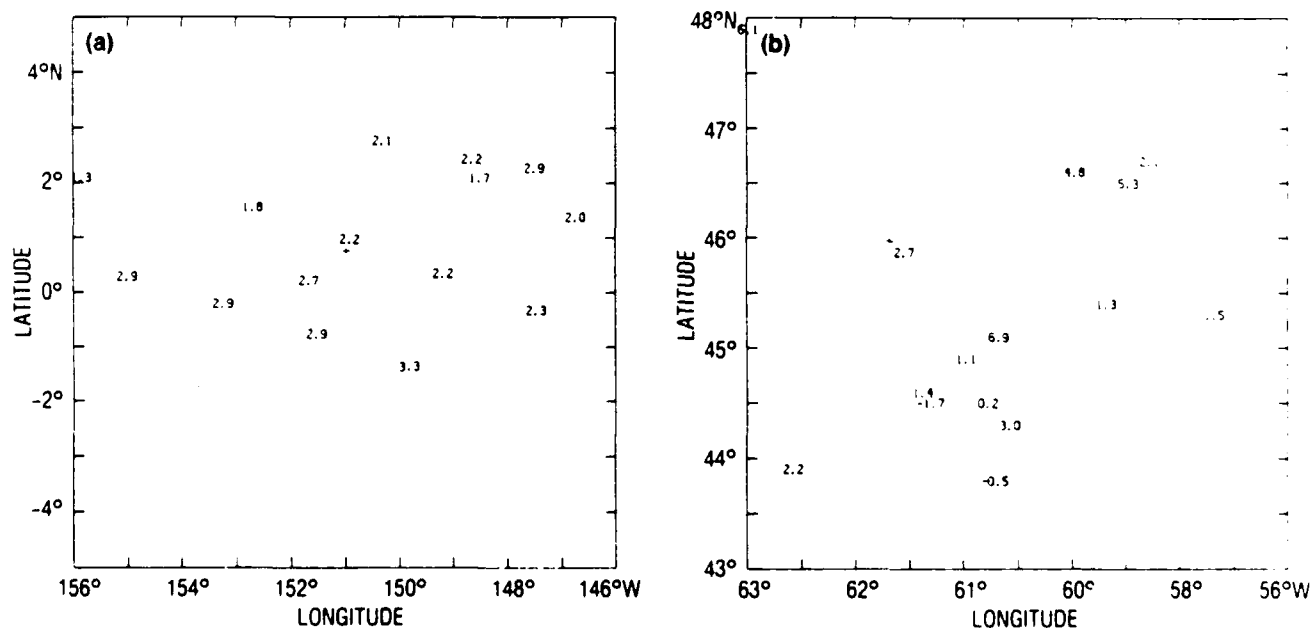


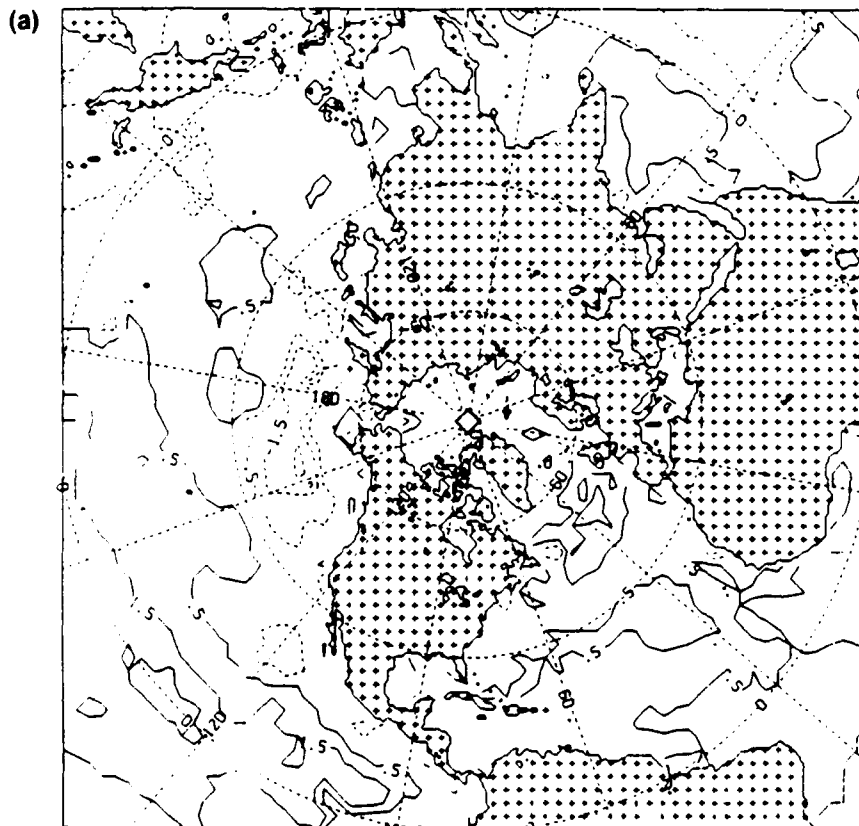
Figure 14. Temperature anomalies selected by the OTIS hemispheric analysis (a) for the grid point located at 1.0°N, 151.0°W, and (b) for the grid point located at 45.9°N, 61.6°W.

Table 5. Quality control of residuals at 45.9°N, 61.6°W.

LAT (°N)	LON (°W)	RESID (°C)	DATA TYPE	REJECTED				
				CASE 1	CASE 2	CASE 3	CASE 4	CASE 5
45.87	61.57	2.65	MCSST	*	*			
45.10	60.70	6.89	SHIP	*	*	*		
44.90	61.00	1.08	SHIP					
46.60	60.00	4.76	SHIP	*	*			*
44.60	61.40	1.41	SHIP					
44.50	61.30	-1.72	SHIP	*	*	*	*	*
45.40	59.70	1.30	SHIP					
44.50	60.80	0.22	SHIP	*	*			
46.50	59.50	5.26	SHIP	*	*			*
44.30	60.60	2.95	SHIP	*	*			
46.70	59.30	2.05	SHIP					
45.30	58.70	1.50	SHIP					
43.90	62.60	2.23	SHIP	*				
43.80	60.70	-0.48	SHIP	*	*	*	*	*
47.90	63.00	6.09	SHIP	*	*			*
ANALYZED	RESIDUAL	CORRECTION	(°C)	0.30	0.36	1.15	1.35	0.94

results in a widely disparate group of observed anomalies (Fig. 14b). Surveying this set of data, not much agreement appears between any of the residuals. The approach taken by the original buddy check is just to throw the majority of the data away (Table 5). However, the analysis should be able to smooth this information intelligently, weighting the observations

by their correlation with the analysis point and according to their respective instrument errors. Table 5 displays the outcome of the five buddy check cases. Note that case 3 removes the apparently erroneous 6.9°C residual, while analyzing one of the largest corrections at the grid point. Considering the input data, this case appears to be the most suitable of the five.



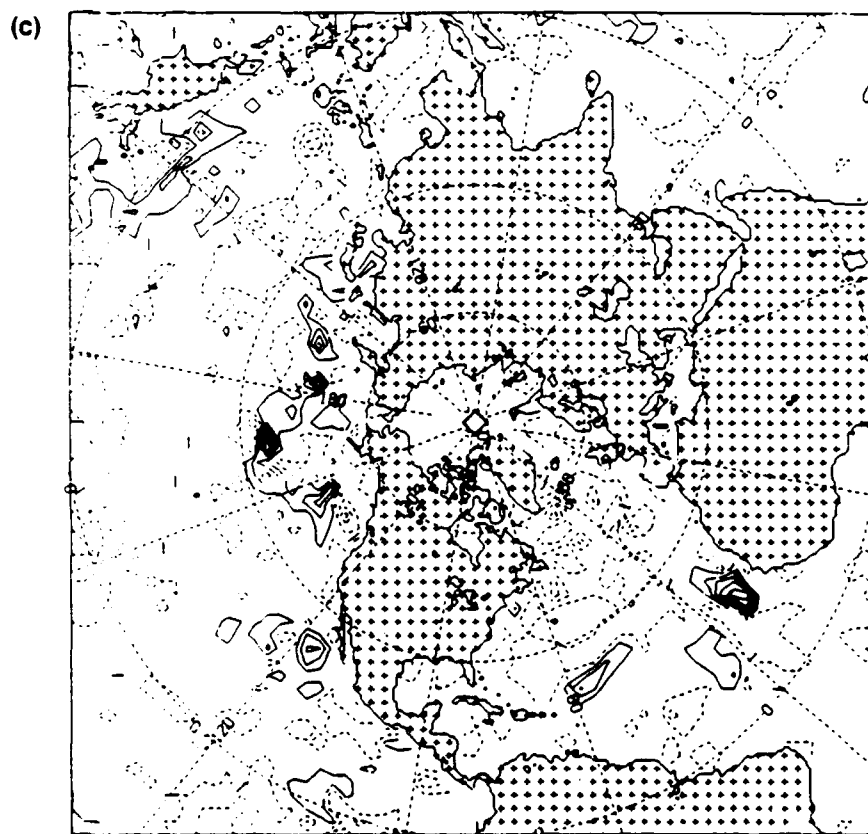
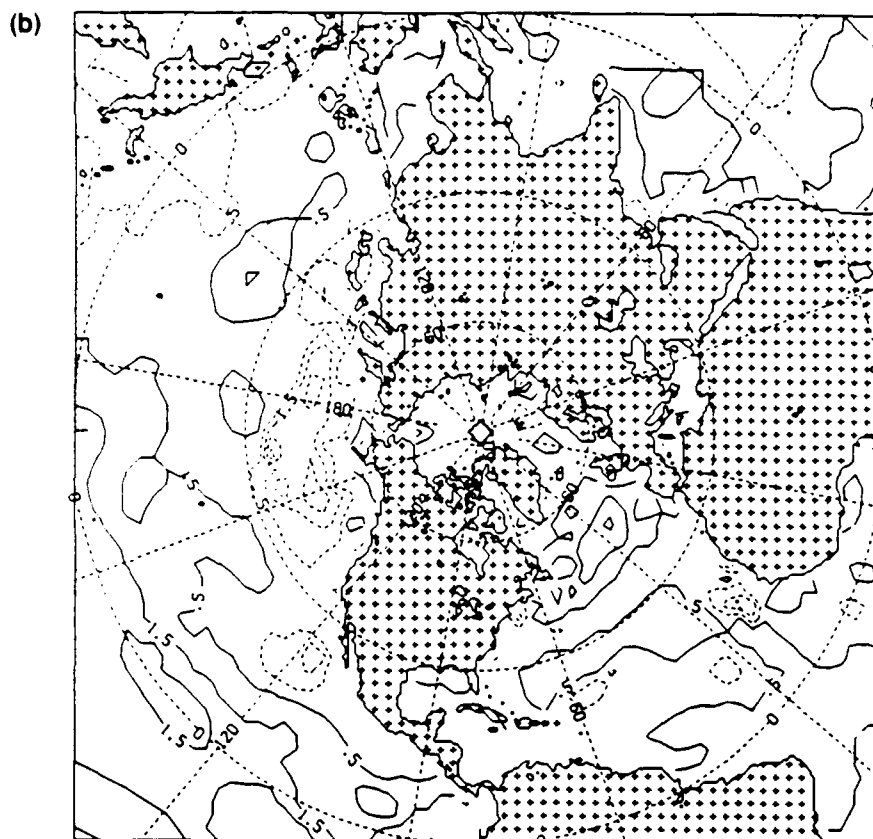


Figure 15. (a) Analyzed anomalies for August 3, 1987, analysis using original buddy check. Contours are every 0.5°C . (b) Analyzed anomalies for same analysis, using buddy check where both keep and toss flags are set on both observations. (c) Difference between the analyses produced in (a) and (b).

Because of these results and other considerations, the buddy check implemented in OTIS 1.0 is the buddy check used in experiment 3. Since the hemispheric OTIS 1.0 creates superobs from the MCSST data and does not distinguish between ship and buoy data (as these tests do), we were concerned that the flagging hierarchy would not work especially well, and that the relatively few MCSST superobs would reject too many of the ship and buoy reports, which are assigned larger errors.

The impact of the quality control changes on the hemispheric SST analysis are revealed in Figure 15, which shows the analyzed SST anomalies from both the original buddy check case (Fig. 15a) and the buddy check later implemented in OTIS 1.0 (Fig. 15b). The difference between the two analyzed fields is shown in Figure 15c. Notice that the largest differences are in the regions where the original buddy check rejected a large percentage of the data (Fig. 11), and that some temperature differences are as large as 2°C.

The same five experiments were repeated for a regional Gulf Stream analysis using data from March 30, 1988. With 2 days of surface data and without creating MCSST superobs, there were 9 XBTs, 306 ship/buoy observations, and 12,443 MCSSTs within the grid area. The buddy check results are again represented by histograms, as shown in Figures 16 and 17. The results from the Gulf Stream OTIS buddy check were similar to the hemispheric case, with the largest improvement stemming from the addition of keep flags. The total number of observations rejected in each case is given in Table 2. Note that for the regional application, case 5 results show an improvement over case 4. This difference between the hemispheric and regional results is likely due to the fact that the MCSSTs are superobs created in the former, but not in the latter. Thus, for regional analyses, the buddy check algorithm used in case 5 appears to be the best choice.

This conclusion is further substantiated by the changes in the Gulf Stream SST analyses made from the March 30, 1988 data. Figure 18a is a plot of the analysis made with the original buddy check in place; Figure 18b is the analysis produced in the fifth experiment. The latter case not only retains more of the observations, but it also results in a more realistic analysis of the south wall of the Gulf Stream. Furthermore, the analysis in the Sargasso Sea is smoother, again reflecting the more consistent data handling algorithm.

VI. Conclusions

During the course of NORDA's work integrating MCSSTs into the various versions of OTIS, it was observed that the automated quality control procedures

were discarding an excessively large number of observations. The gross-error check, which determines the allowed deviation an observation can have from climatology, was too restrictive and rejected all anomalies larger than 5°C. This criterion almost guarantees that the analyzed fields will look very much like climatology. Based on several case studies, the gross-error checks have been relaxed to 7°C in OTIS 1.0 and 10°C in the regional SST-OTIS.

The different values for hemispheric versus regional analyses reflect the fact that the acceptable anomaly must be a function of the scales to be analyzed. Furthermore, in the ideal situation, the gross-error check should also be a function of the particular location of the observation. This variation would allow less restrictive criteria to be used in areas of extremely cold upwelling and dynamically active regions of the oceans, without permitting bad data to pass through in areas where little deviation from climatology would be expected. FNOC is pursuing this idea and should implement it in the future.

Relaxing the gross-error check makes it even more important to apply the buddy check properly if erroneous observations are to be identified and removed. Experiments with both regional and hemispheric analyses clearly demonstrated that the original buddy check design was far too intolerant. Altering the values of some of the empirical constants and adding the use of keep flags for corroborating observations greatly reduced the incidence of data rejection. Other, more subtle, refinements in the buddy check were not implemented in OTIS 1.0, but probably have merit for regional analyses, especially if the MCSST data are not superobed.

One further problem with the buddy check remains. The buddy check implemented in OTIS 1.0 and described by Bergman (1979) is a point-by-point procedure; that is, only the data selected for the analysis at each point are actually screened. Such a procedure has the advantage of being fast, since it checks only the data input to the analysis and therefore has to search the data only once per grid point. However, it also has the undesirable capability of excluding an observation at one point while accepting and using it at the next. Because this is a potential source of noise in the analysis, NMC later chose to perform all data screening prior to beginning the actual analysis, and to design the system in such a way that each observation was guaranteed to be included in at least one group (Kistler and Parrish, 1982).

During discussions with FNOC, NORDA suggested that all quality control of the data in OTIS be done prior to the actual analysis. This way, the rejected observations are permanently removed from the data set and are not included in the analysis at any point. However, because of the major software changes required to accomplish such a task, no action has been

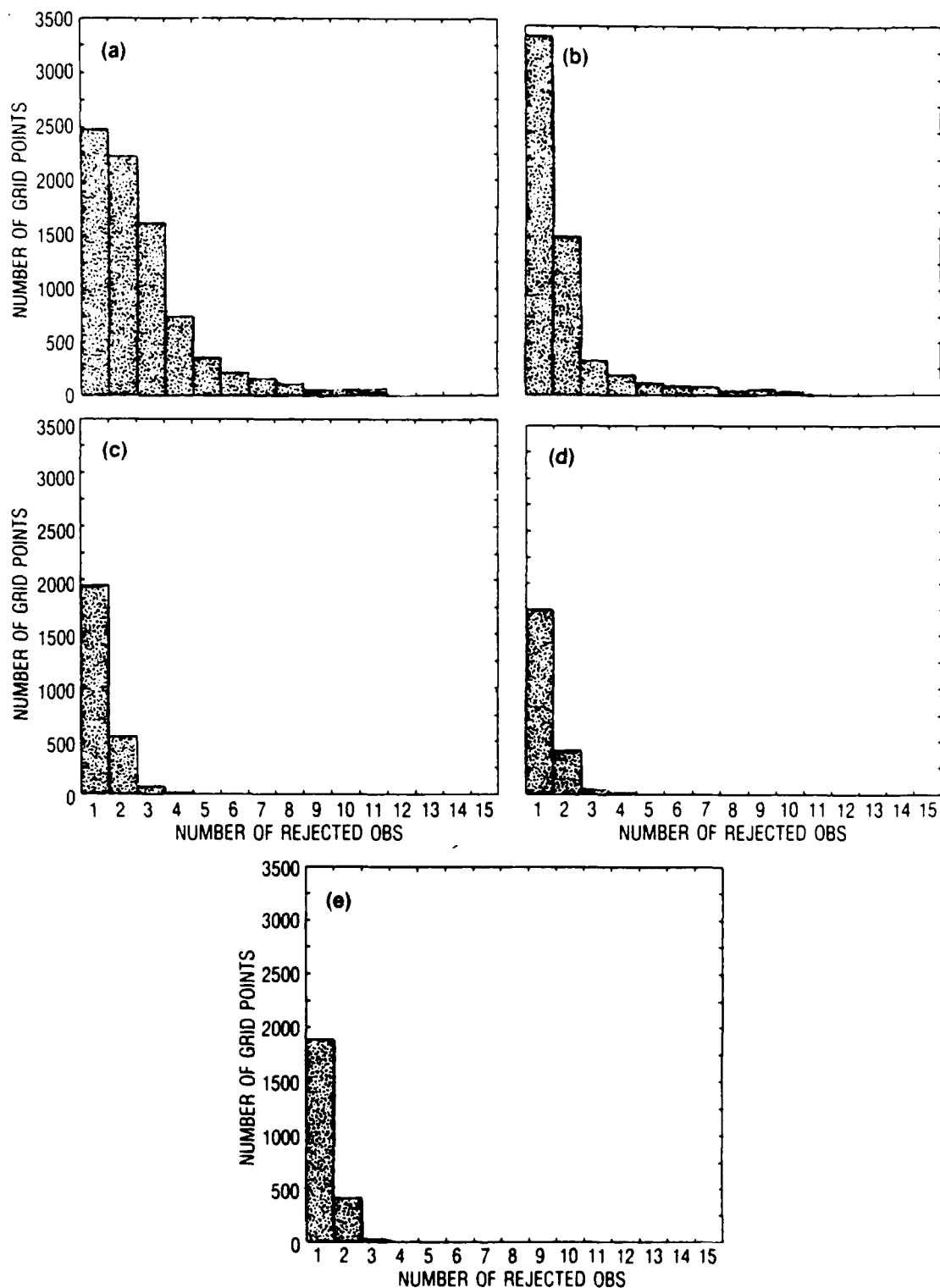


Figure 16. Histograms illustrating how many of the 15 selected observations were rejected by the buddy check, and at how many grid points this situation occurred for the regional Gulf Stream analysis on March 30, 1988. (a) Original buddy check; (b) constants a and b increased by 50%; (c) keep flags, as well as toss flags, set on both observations; (d) keep flags set on both observations, but toss flags set on only one; (e) autocorrelation used as flag value and flag limits reduced to 1.5.

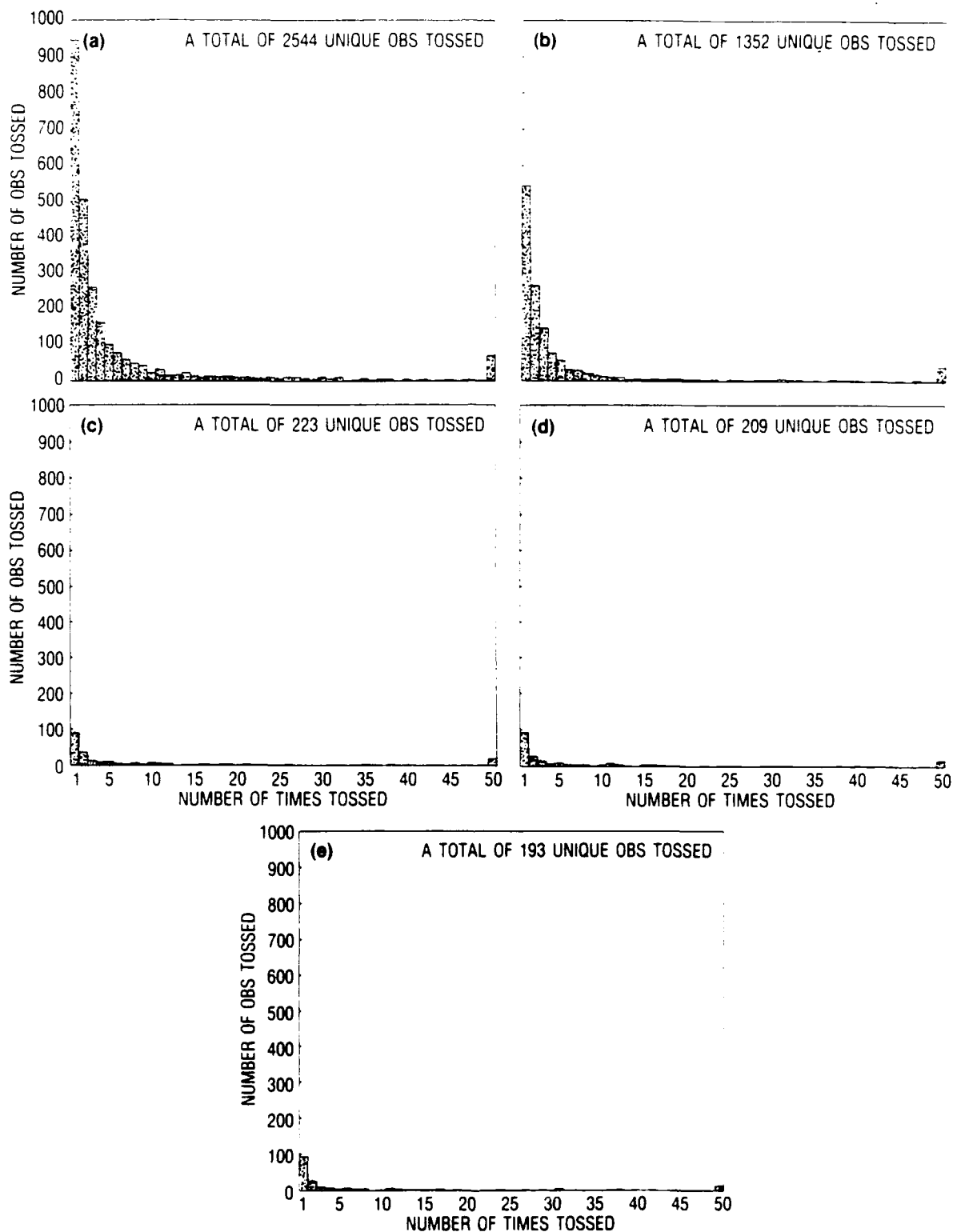


Figure 17. Histograms illustrating how many times a particular observation was rejected, and the number of observations in each of these categories for the regional Gulf Stream analysis on March 30, 1988. (a) Original buddy check; (b) constants a and b increased by 50%; (c) keep flags, as well as toss flags, set on both observations; (d) keep flags set on both observations, but toss flags set on only one; (e) autocorrelation used as flag value and flag limits reduced to 1.5.

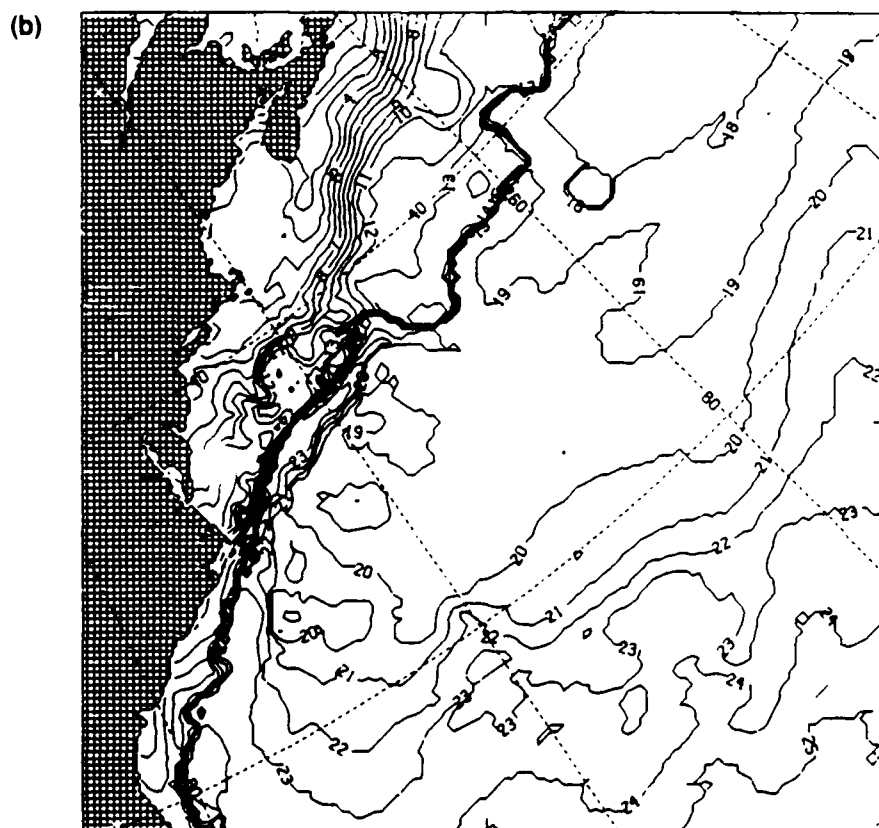
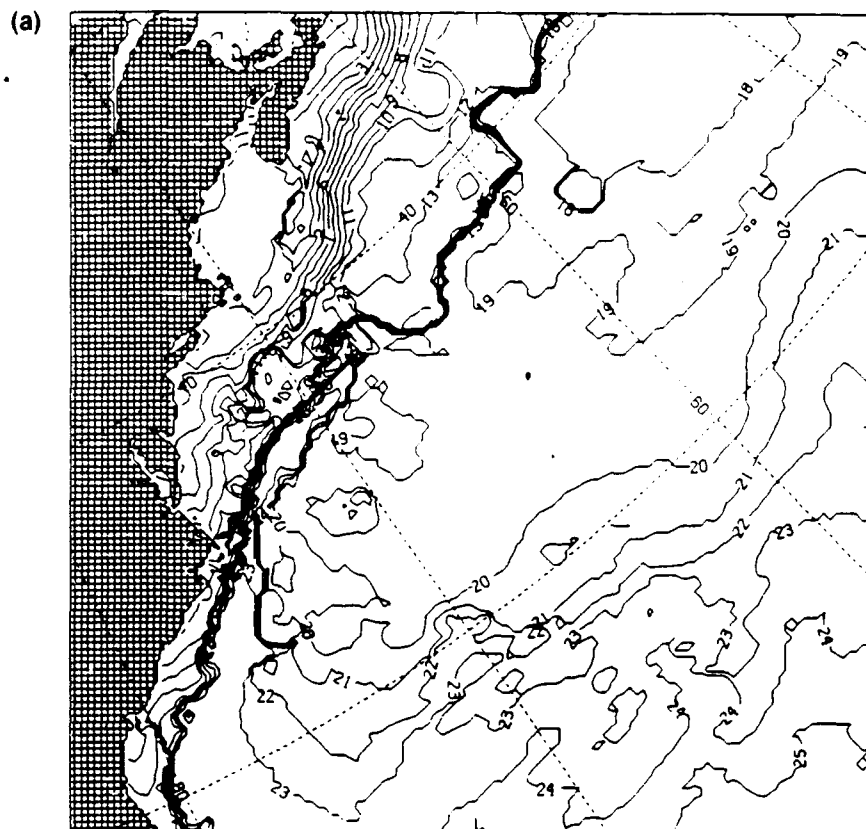


Figure 18. OTIS 20-km Gulf Stream SST analyses. (a) Original buddy check; (b) modified buddy check, including all case 5 options.

taken along these lines in OTIS 1.0. Also, at the time, the point-by-point buddy check did serve a useful purpose. At grid points near the boundaries of mesoscale features, where strong gradients exist, the buddy check could effectively decorrelate data across those boundaries by rejecting the large anomalies that would be present in the other water mass.

Several later changes make this idea much less effective. First, the anomalies on the other side of the mesoscale boundaries were large because at the time, all anomalies were formed relative to the analysis grid point. That is, once the 15 observations were selected, the first guess valid at the grid point was subtracted from each temperature observation. This oversight results in an observation with a different anomaly value for every analysis point using that observation. Such a definition directly contradicts the theory of optimum interpolation, which requires that the first guess be interpolated from the gridded field to the location of each observation and subtracted from the observed value to form the anomaly. This error has now been corrected, making the buddy check less effective for decorrelating separate water masses.

Furthermore, for regional analyses where mesoscale features play an important role, a separate technique has been designed to decorrelate data across these front and eddy boundaries (STX, 1987). During the data selection process, only observations that are in the same water mass as the analysis grid point can be considered. Therefore, the anomalies that are buddy checked together at a point are always considered to be in the same water mass. Thus, the arguments to keep the buddy check within the analysis are now less relevant.

The next generation of regional OTIS, called OTIS 2.0, became operational in the Gulf Stream area in June 1989. This version of OTIS corrects some of the previous problems with quality control in OTIS 1.0. In particular, it does all the quality control before the analysis begins. It also uses a sophisticated technique whereby optimum interpolation is used to perform the horizontal consistency check. In this approach, an optimum interpolation analysis is made at the location of each questionably large anomaly using all the neighboring observations, but not the data point in question. This analyzed value is then compared to the excluded observation, and if the deviation is not too large, then the observation is allowed to remain (J. Cummings, Fleet Numerical Oceanography Center, pers. comm., 1989). This method has been used by the Naval Environmental Prediction Research Facility and others for quality control of meteorological data, and has proven to be very successful. It is, however, more demanding of computer resources and thus may not be practical for all applications.

VII. Recommendations

In summary, the changes made to the quality control and data selection procedures in OTIS 1.0 resulted in an analysis that was faster, more accurate, and verified better against independent data sources (R. M. Clancy, Fleet Numerical Oceanography Center, pers. comm., 1989). These experiments have further demonstrated that quality control of the available data is extremely important. Additionally, more sophisticated, automated procedures should be developed to intelligently handle the vast amounts of data that must be checked. Since the analysis is a reflection of the input data, it is crucial that erroneous observations are not allowed to have an undue influence on the final product.

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13. Abstract (Maximum 200 words). The Fleet Numerical Oceanography Center (FNOC) provides daily analyses of the three-dimensional ocean thermal structure both to the Fleet and to regional oceanography centers around the world. These analyses are performed on both hemispheric and regional scale grids, with resolutions as fine as 20 km in some areas. The Remote Sensing Branch of the Naval Ocean Research and Development Activity (NORDA) has been involved in assessing the impact of multichannel sea surface temperatures (MCSSTs) on these ocean thermal analyses. Specifically, NORDA has worked closely with FNOC in developing the Optimum Thermal Interpolation System (OTIS). NORDA's primary interest was to assure that the MCSSTs were properly utilized to detect and analyze mesoscale ocean fronts and eddies, with particular attention paid to how the MCSSTs were assimilated with other types of data. Through this joint effort, FNOC has successfully implemented OTIS as the operational ocean thermal analysis system for the global analysis and the Gulf Stream regional analysis. In addition to processing and assimilating data from various sources, OTIS includes algorithms to automatically make decisions about the quality of the observations and to ignore data that are apparently erroneous. There are two basic methods of quality controlling data in OTIS. The first is the gross-error check, where observations are compared to the climatological first-guess field to assure that the data fall within reasonable ranges of the expected values. Then, groups of observations are subjected to a check for horizontal consistency, often called a "buddy check." Thus, if a particular observation cannot be corroborated by other nearby data, it is generally excluded from the analysis. This report describes the details of the automated quality control procedures in OTIS, and provides an account of the fine tuning that is necessary to optimize these techniques. The end result is a system that eliminates most of the bad data while retaining most of the valid observations, thus contributing to an improved ocean thermal analysis product.					
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